Thermoelectric properties of semiconductor nanostructures

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Outline

- Intense interest in high-efficiency (ZT~1) semiconductor thermoelectrics for wide range of applications
- Thermal conductivity key to thermoelectric performance
- Thermal conductivity in SOI/nanomembranes
  - Anisotropy and surface scattering
  - Results: comparison to bulk and SOI measurements
- Thermal conductivity in SiGe-based superlattices
  - Interface scattering model for superlattices
  - Results: thermal conductivity in Si/Ge superlattices
  - Results: thermal conductivity in Si/SiGe alloy superlattices
- Conclusions

Model for thermal conductivity

- Compute the full thermal conductivity tensor
- Sum contributions from all phonon branches
- Capture temperature and rms roughness dependence
- Use the full phonon dispersion for phonon energies and velocities

$$\kappa^{\alpha\beta}(T) = \frac{1}{T}\left[L^{(2)}\right]^{\alpha\beta}$$

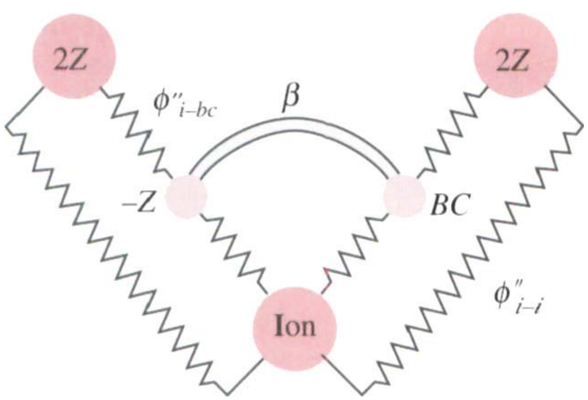
$$\left[L^{(2)}\right]^{\alpha\beta} = \sum_{\mathrm{j}} \int_0^{\omega_{\mathrm{j}}} d\omega \left(\frac{dN_0}{d\omega}\right) \sigma_{\mathrm{b}}^{\alpha\beta}(\omega)\left(\hbar\omega\right)^2$$

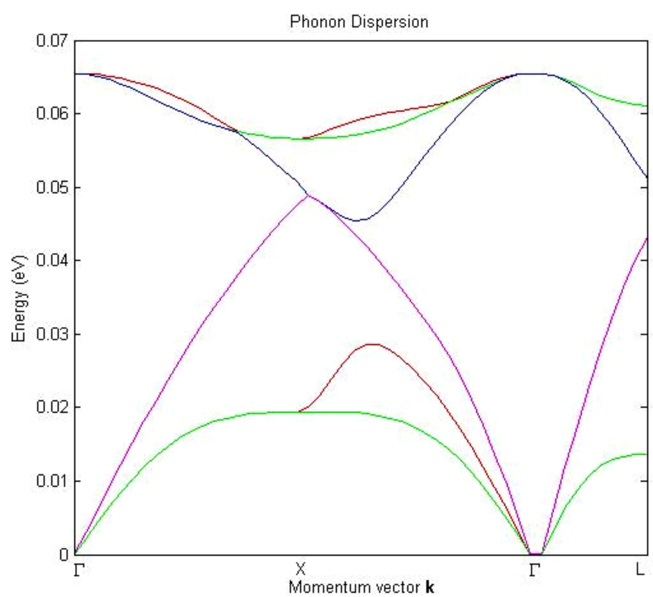
$$\sigma_j^{\alpha\beta}(\omega) = \int \frac{d\vec{q}}{(2\pi)^3} \tau_j(\vec{q}) \vec{v}_j^{\alpha}(\vec{q}) \vec{v}_j^{\beta}(\vec{q}) \delta\left(\omega - \omega_j(\vec{q})\right)$$

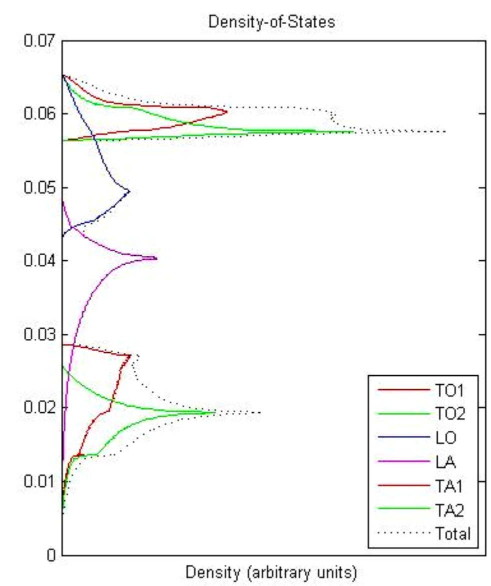
- In a superlattice, the thermal conductivity of the two alternating layers is combined in series for cross-plane transport and in parallel for in-plane transport

Phonon dispersion calculation

- Weber's Adiabatic Bond Charge model[1] is used to calculate the full phonon dispersion throughout the Brillouin zone
- Predicts phonon dispersion of Si and Ge with <2% average error
- Properties of $Si_{1-x}Ge_x$ alloys calculated in the virtual crystal approximation



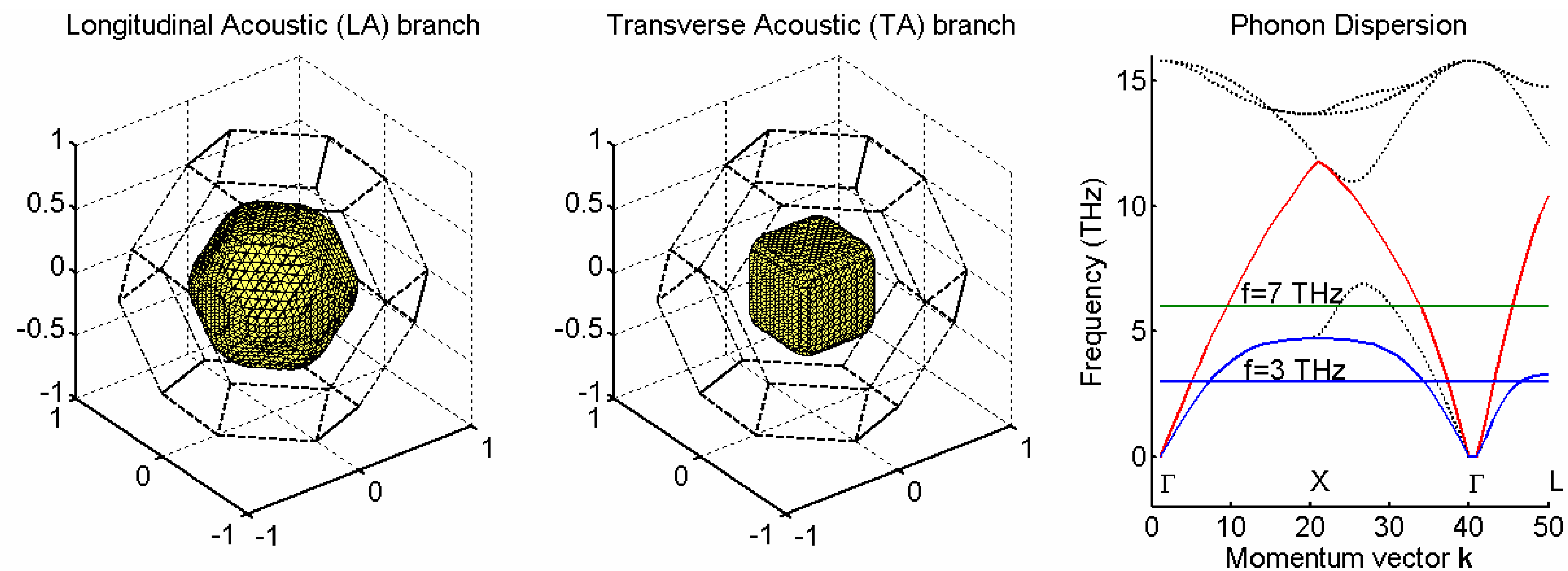




[1] W. Weber: Adiabatic bond charge model for the phonons in diamond, Si, Ge, and α-Sn. Phys. Rev. B **15**, 4789–4803 (1977)

Anisotropy of phonon dispersion

- Phonon isosurfaces show strong anisotropy and phonon focusing
- LA branch (below, left) has very flat faces with surface normals in the [111] direction
- TA branch (below, right) has isosurfaces normal to the [100] direction

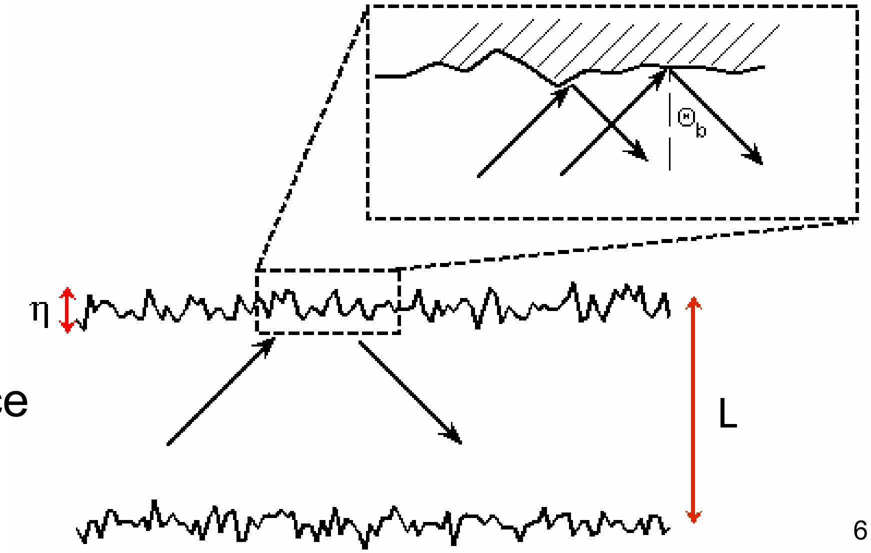


Surface scattering of phonons in semiconductor nanostructures

- Scattering with interfaces/boundaries dominates transport in nanostructures
- Describe the interaction between phonons and surfaces by a specularity parameter 0<=p<1
- At a rough interface, phonons can be reflected (specular, p=1) or scattered in a random direction (diffuse, p=0)
- Momentum-dependent specular-diffuse interface scattering parameter p(q) dictates surface interactions:

$$p(\vec{q}) = \exp(-4q^2\Delta^2\cos^2\Theta_B)$$

- Allows us to connect specularity parameter to phonon momentum, rms roughness and angle of incidence



Phonon lifetime and mean-free-path due to scattering with boundaries

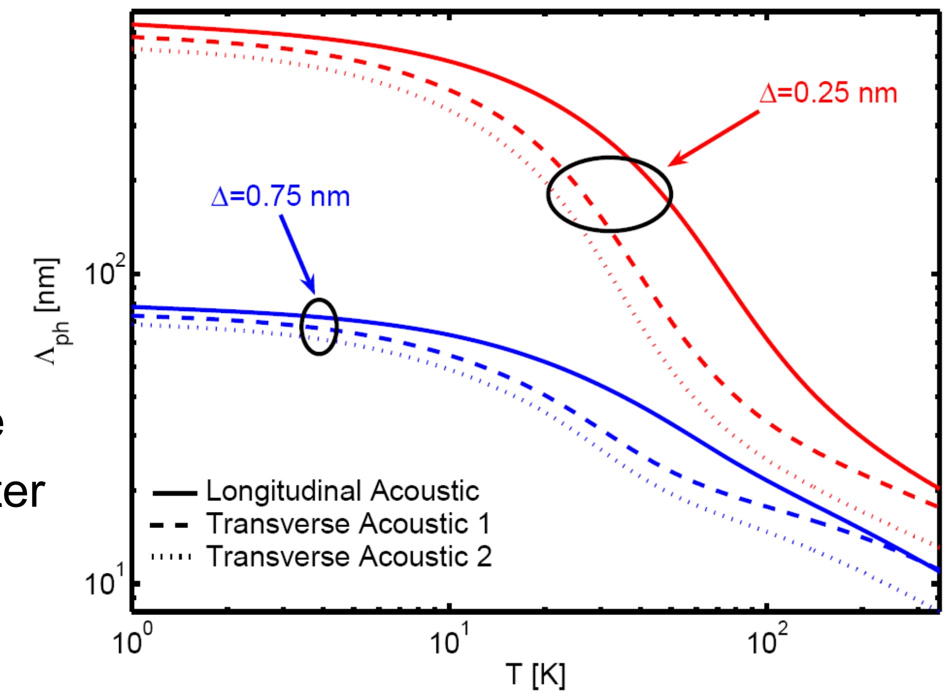
- Mean-free-path is the distance that the phonon travels between surface scatterings:

  $(1-p)L+3p(1-p)L+5p^2(1-p)L+7p^3(1-p)L\ldots=(1+p)/(1-p)L$

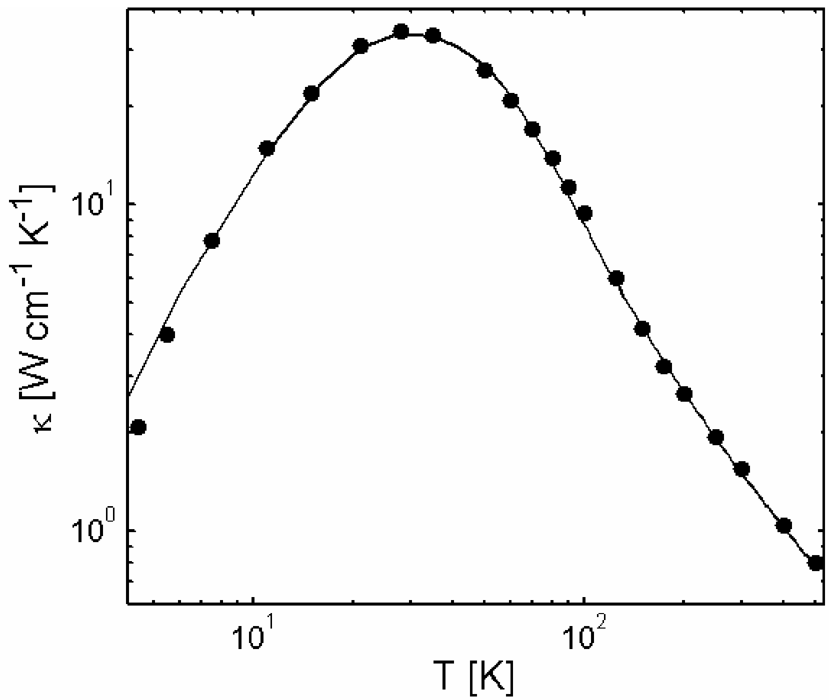
- Phonon lifetime due to boundaries is then given by the ratio of distance between boundaries (L) and the phonon velocity in the direction of surface normal ($v_\perp$):

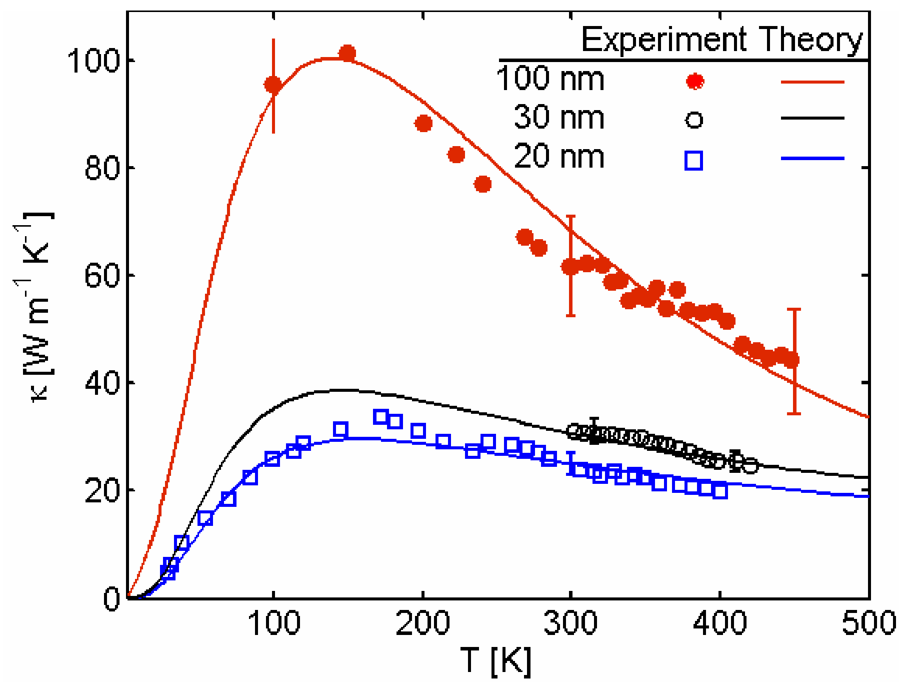
$$\tau_b(\vec{q}) = \left(\frac{1+p(\vec{q})}{1-p(\vec{q})}\right)\frac{L}{v_\perp(\vec{q})}$$

- Phonon mean-free-path depends on rms roughness and temperature because of the specularity parameter



Bulk silicon and ultrathin SOI: comparison with experiments

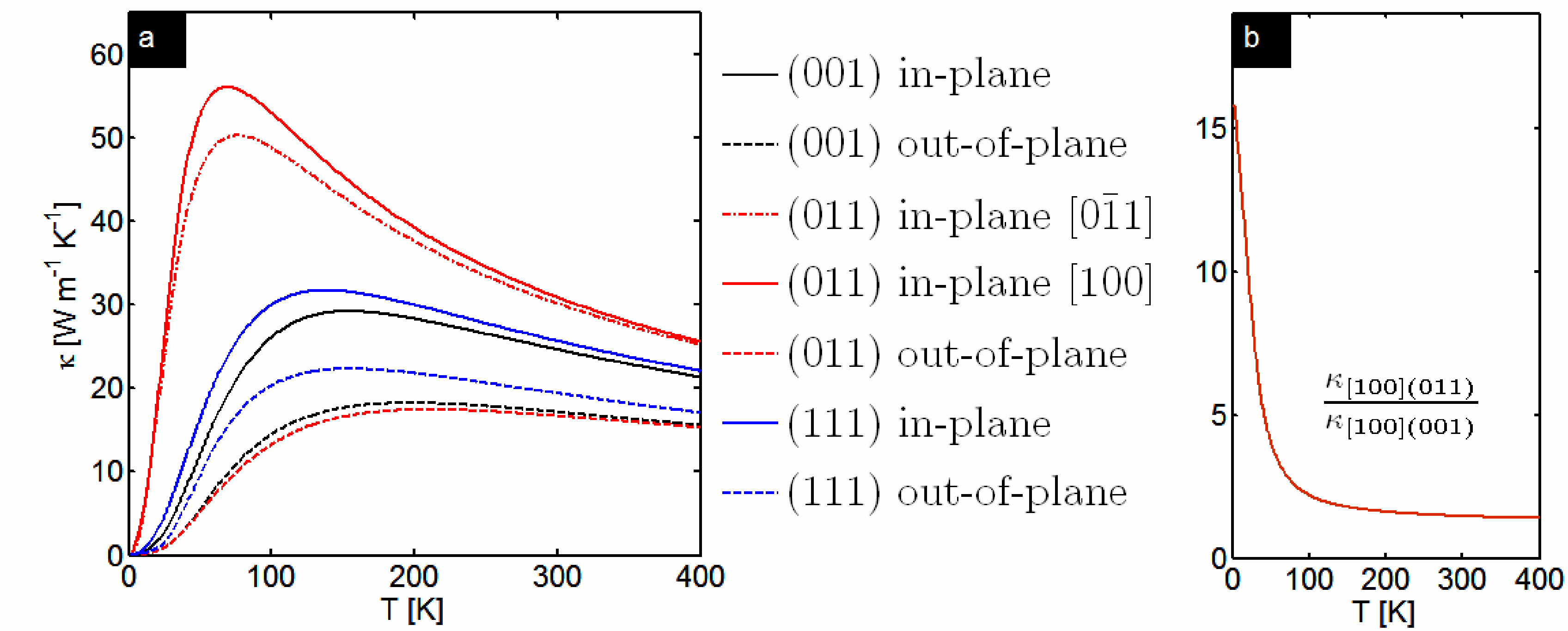




- Good agreement with measurements of bulk silicon thermal conductivity over a wide range of temperatures (Glassbrenner and Slack, Phys. Rev. 134, A1058-A1069 (1964))
- Good agreement with measurements of thermal conductivity in 20, 30, and 100 nm SOI (Liu and Asheghi, JHT 2006)

Anisotropic thermal conductivity in ultrathin silicon

- Computed thermal conductivity in 20nm SOI shows strong anisotropy
- Lowest thermal conductivity is on a (001) surface
- Highest thermal conductivity achieved on (011) surface
- Overall ratio of highest and lowest in-plane thermal conductivity is roughly a factor of 2 at room temp. and higher at low temperature
- Allows additional control over thermal conductivity



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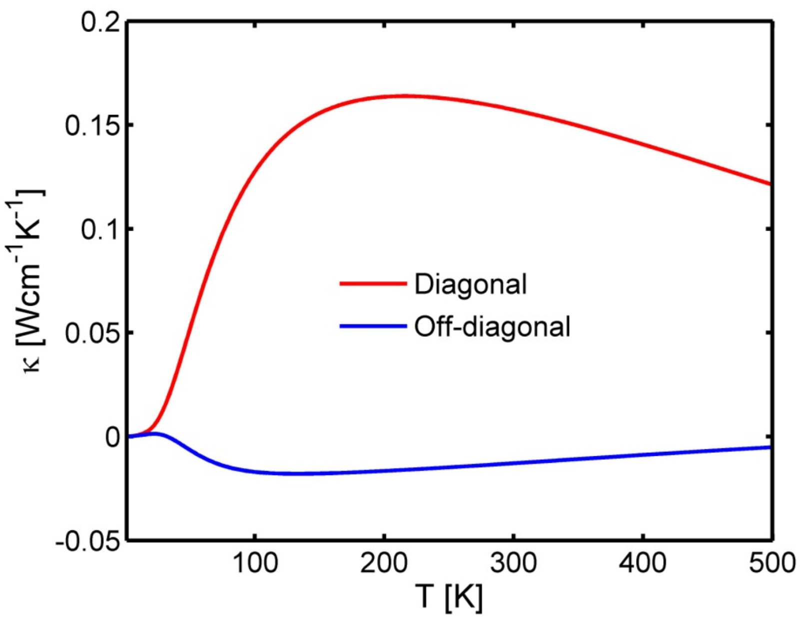
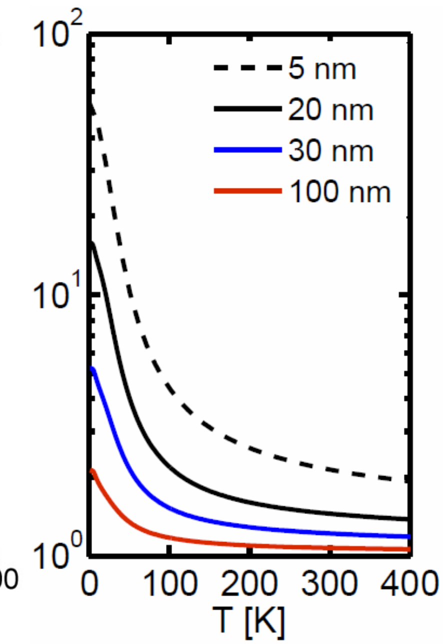
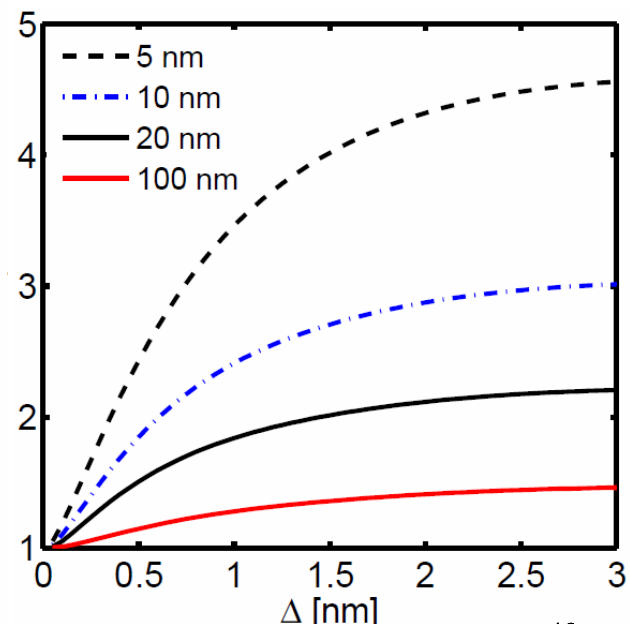
Thermal conductivity tensor in ultrathin silicon nanomembranes

- 3x3 thermal conductivity tensor has distinct diagonal and off-diagonal components at each temperature
- 3 eigenvalue/eigenvector pairs:
  - 1 eigenvector in the direction of the surface and 2 in-plane
- Eigenvectors independent of temperature, only depend on surface orientation
- In/out-of-plane and highest/lowest in-plane ratios both depend on thickness and rms surface roughess







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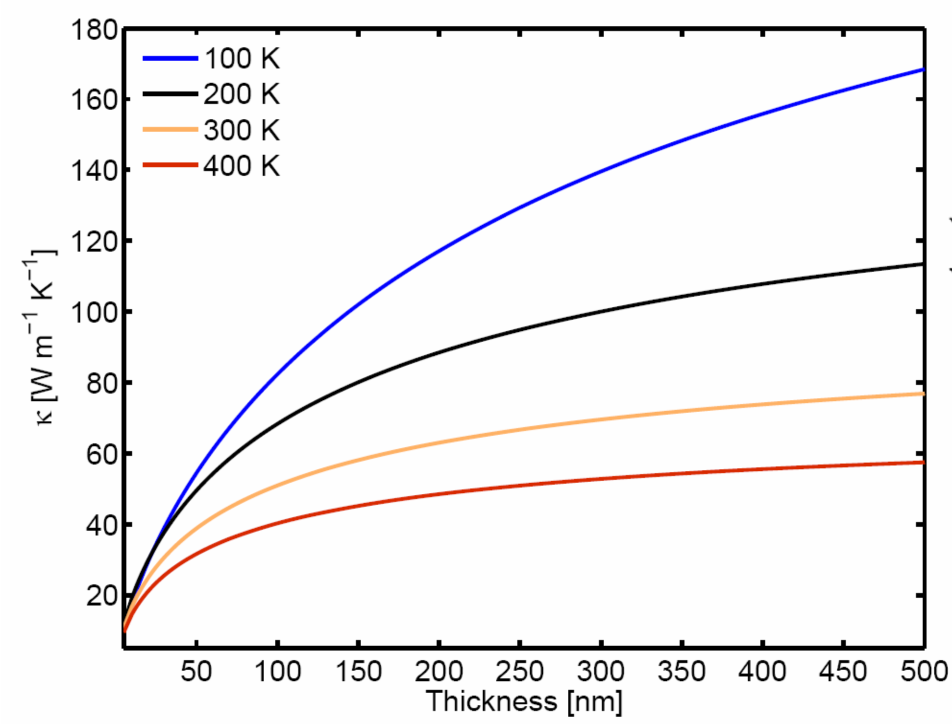
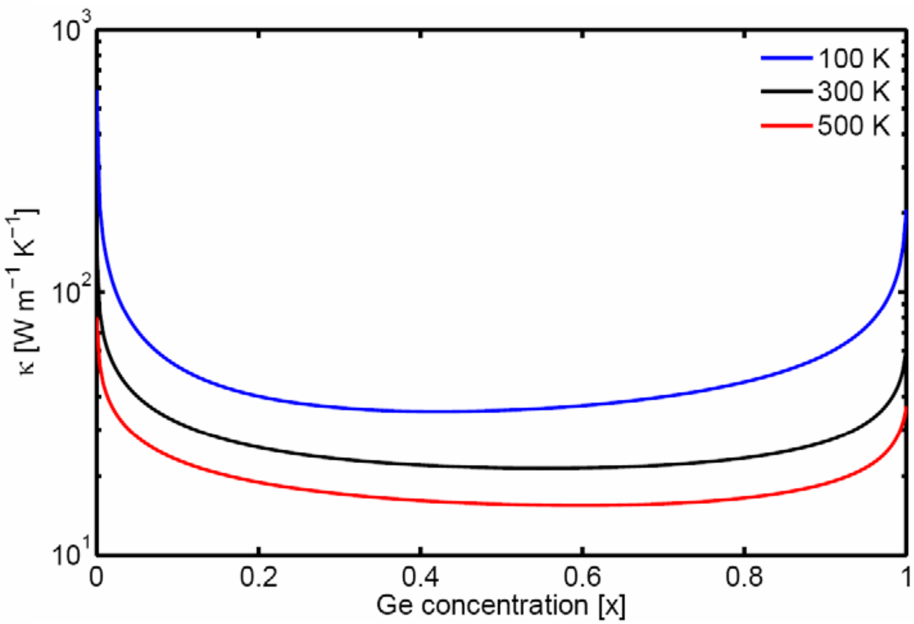
Thickness and composition dependence of thermal conductivity

- Strong dependence on thickness in the sub-50nm regime
  - boundary scattering dominates
- Bulk alloys also show strong dependence on composition and reach a plateau for a broad range (0.1<x<0.9) of compositions
- Both nanostructuring and alloying reduce thermal conductivity by roughly an order of magnitude



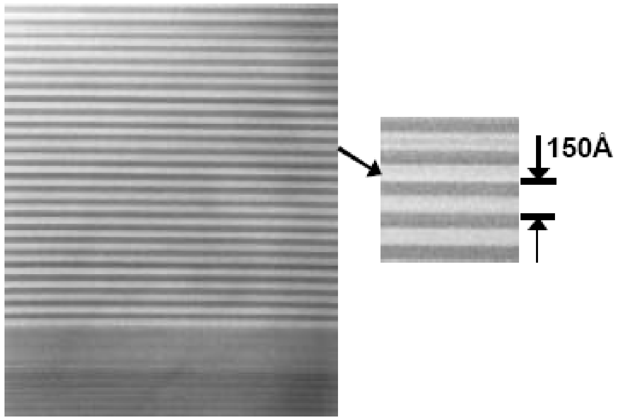


Specularity parameter in superlattices

- Superlattices are made up from many thin layers of alternating semiconductor materials
- Each layer is only a few nanometers thick
- Layers are separated by a rough interface described by an average rms rougness parameter
- Average the single-interface momentum-dependent scattering parameter p(q) over some distribution P of roughness heights:

$$p(\vec{q}) = \int_0^\infty P(\Delta) \exp\left(-4\pi^2\Delta^2 q^2 \cos^2\Theta\right) d\Delta$$

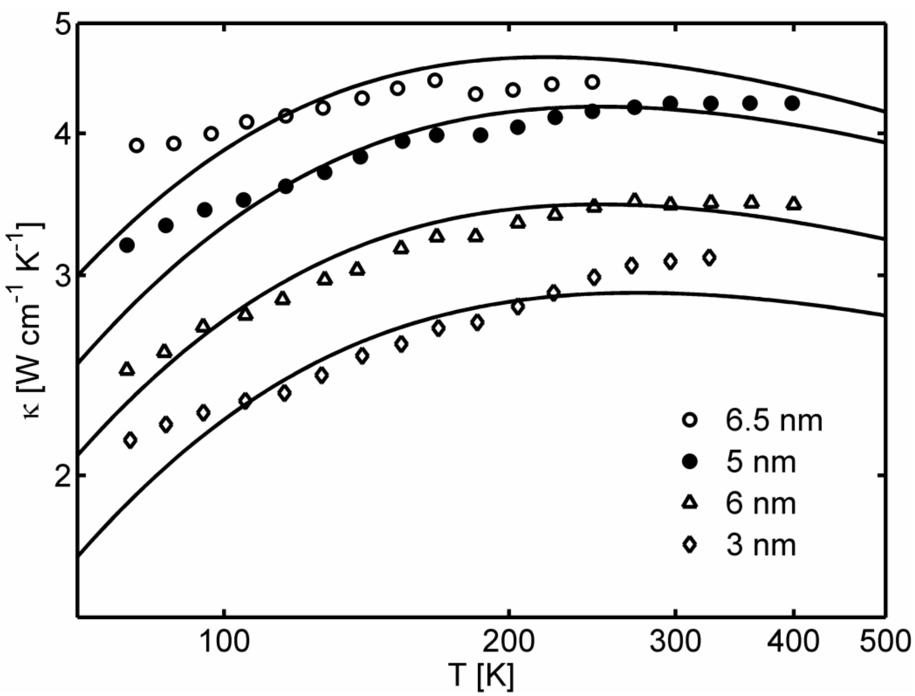
- Average specularity parameter depends on phonon momentum, average roughness and angle of incidence



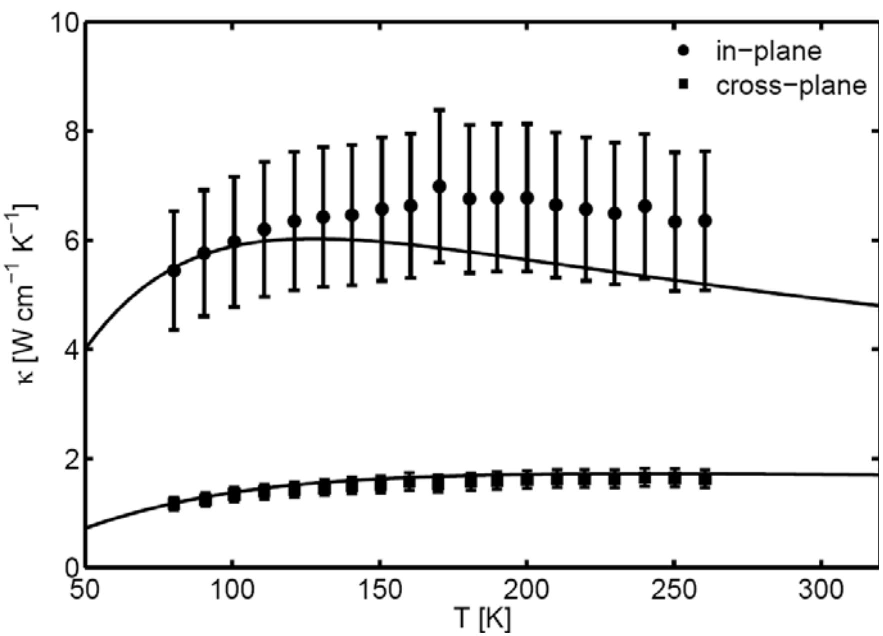
SEM image from
S. T. Huxtable, Ph.D. Thesis

Thermal conductivity of Si/Ge superlattices

- Treat superlattices as alternating thin nanomembranes in series
- Strong in-plane/cross-plane anisotropy
- Very low (1~5 W/m/K) cross-plane (along the superlattice) thermal conductivity



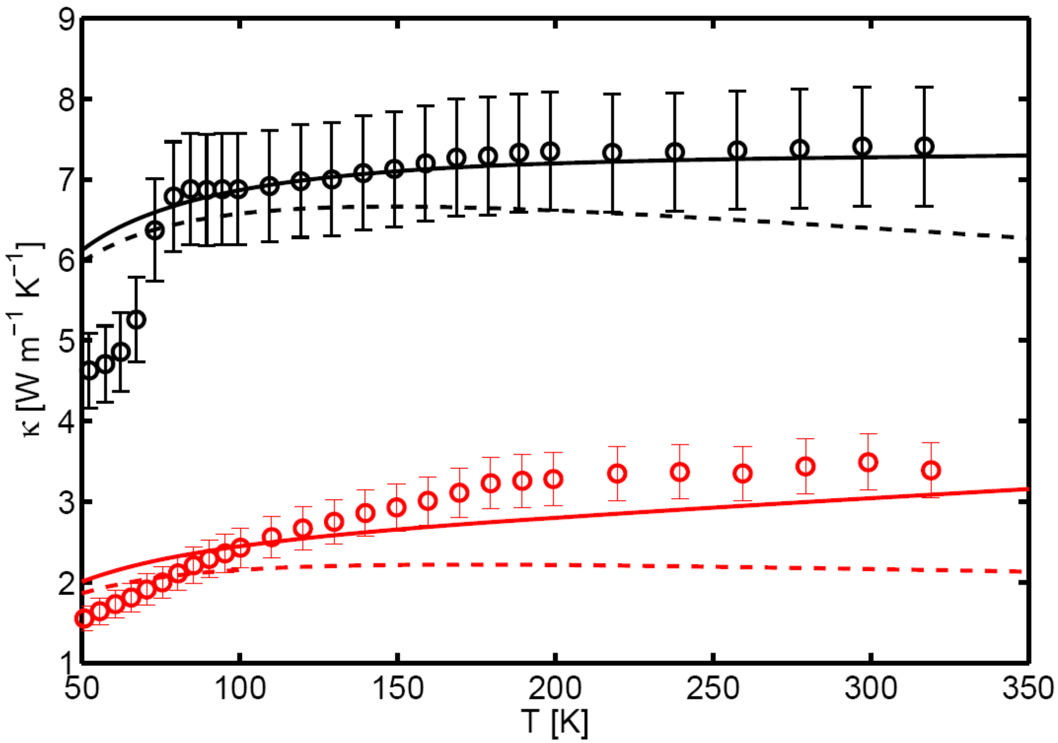
Lee, et al. Appl. Phys. Lett. **70**, 2957 (1997)



Liu, et al. J. Nanosci. Nanotech. **1**, 39 (2001)

Thermal conductivity of $Si_{1-x}Ge_x$ alloy films and $Si/Si_{1-x}Ge_x$ SLs

- Black: 3.5um $Si_{0.3}Ge_{0.7}$ alloy film
- Red: 15nm $Si_{0.4}Ge_{0.6}$ alloy superlattice
- Superlattice thermal conductivity below alloy limit
- Can be explained by scattering of phonons from rough interfaces between layers



S. T. Huxtable et al. Appl. Phys. Lett. **80**, 1737 (2001)

Conclusions

- Thermal conductivity is key to thermoelectric performance
- Thermal conductivity is strongly dependent on the properties of surfaces, boundaries, and interfaces
- In silicon nanomembranes and thin SOI, thermal conductivity shows strong anisotropy, with highest in-plane thermal conductivity on (011) and lowest on (001) surfaces
- In-plane/out-of-plane ratio is also very high on all surfaces and increases with lower thickness and higher roughness
- Thickness and composition dependence can be utilized to lower thermal conductivity in alloy films and superlattices
- Anisotropy also observed in superlattices

Acknowledgement

- This work has been supported by the Computing Research Association and by the National Science Foundation (award No. 0937060) through a Computing Innovation Fellowship, subaward No. CIF-146, and the AFOSR (YIP program, award No. FA9550-09-1-0230).

- Questions?